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Research Article

Extremal Zagreb indices of a tree with given double Roman domination number

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Abstract: In this article, some upper and lower bounds for the first and the second Zagreb indices of an arbitrary tree in terms of its order and double Roman domination number γ_{dR}, (depending on whether γ_{dR} is odd or even), are stated. Also, all extremal trees attaining equality are characterized.

Keywords: double Roman domination number, double star, path, star, tree, Zagreb indices.

AMS Subject classification: 05C09, 05C05, 05C69

1. Introduction

Let $G = (V(G), E(G))$ be a tree with the vertex set $V(G)$ and the edge set $E(G)$. The *order* of G refers to the number of its vertices. The *open neighborhood* of a vertex v is the set $N(v) = \{u \in V(G) \mid uv \in E(G)\}$ and the *closed neighborhood* of v is the set $N[v] = N(v) \cup \{v\}$. The *degree* of a vertex $v \in V$ is $d(v) = |N(v)|$. The maximum degree of G is represented by Δ. A *leaf* is a vertex of degree 1 and a *support vertex* is a vertex adjacent to a leaf. For any two distinct vertices u and v, the number of edges in a shortest path connecting them is called their distance and is represented by $d(u, v)$. The *diameter* of G, denoted by $diam(G)$, is the greatest distance between two vertices of G. A diametral path is the shortest path between two vertices u and v with $d(u, v) = diam(G)$. We write P_n and S_n for the *path* and the *star* of order n, respectively. The *double star* $DS_{p,q}$ is

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a tree obtained from S_{p+1} and S_{q+1} by connecting the center of S_{p+1} with that of S_{q+1}.

In mathematical chemistry, topological indices are numerical values that are invariant under graph isomorphism and are used to describe the physicochemical structures of molecules. Among the topological indices based on vertex degree, the *first* and *second* Zagreb indices have garnered considerable interest. These indices were first introduced in 1972 by Gutman and Trinajstić [10] and they have a good correlation with certain chemical properties. For an arbitrary graph G, they are defined by the following formulas:

$$M_1(G) = \sum_{v\in V(G)} d^2(u) = \sum_{uv\in E(G)} d(u) + d(v) \quad , \quad M_2(G) = \sum_{uv\in E(G)} d(u)d(v)$$

A considerable amount of research has been conducted on the Zagreb indices. Some results for the Zagreb indices can be found in [6, 9, 13] and the references therein.
A *double Roman dominating function* (shortly, *DRDF*) on a graph G is a function $f : V(G) \to \{0, 1, 2, 3\}$ having the property that if $f(u) = 0$, then the vertex u has at least two neighbors assigned 2 under f or one neighbor w with $f(w) = 3$, and if $f(u) = 1$, then the vertex u must have at least one neighbor w with $f(w) \geq 2$. The minimum weight, $w(f) = \sum_{v\in V(T)} f(v)$, of double Roman dominating functions on T is defined as the *double Roman domination number*, of T and is denoted by $\gamma_{dR}(T)$. A double Roman dominating function with weight $\gamma_{dR}(T)$ is referred to as a γ_{dR}-function (see [1] and [5]) .

Recently, the relationship between topological indices of trees and types of their dominating sets has been studied. For example, in papers [7, 12], the connection between Zagreb indices and the domination number of trees has been explored. Additionally, in papers [2–4, 8], bounds for Zagreb indices of trees have been derived using the Roman domination number. In this paper, upper and lower bounds for the Zagreb indices of a tree are provided by using its double Roman domination number.

2. Preliminaries

We start this section by stating the Zagreb indices and the double Roman domination number of P_n's which will be useful in proving the results of the article. Calculating the mentioned parameter and indices is straightforward.

Lemma 1. *Let $n \geq 2$ be an integer number. Then $M_1(P_n) = 4n-6$ and $M_2(P_n) = 4n-8$.*

Lemma 2. *[1, Proposition 1] Let n be a positive integer number. Then*

$$\gamma_{dR}(P_n) = \begin{cases} n & n \equiv 0 \pmod 3 \\ n+1 & n \equiv 1, 2 \pmod 3 \end{cases}$$

The following upper bound for the double Roman domination number of a tree (an arbitrary graph) in terms of its order and its maximum degree was stated in [11].

Lemma 3. *[11, Theorem 3] Let G be a graph of order n and maximum degree Δ. Then*

$$\gamma_{dR}(G) \leq 2n - 2\Delta + 1$$

Lemma 4. *Let T be a tree of order n and u is a leaf in T. Then*

$$\gamma_{dR}(T-u) \leq \gamma_{dR}(T) \leq \gamma_{dR}(T-u) + 2.$$

Proof. The proof is straightforward. □

Definition 1. The graph $S_{n,k}$ is a graph of order n, that has one vertex of degree $n-k-1$, k vertices of degree 2 and $n-k-1$ vertices of degree 1. In other words, the graph $S_{n,k}$ is obtained from the star S_n by adding k pendant edges to some its leaves (see Figure 1).

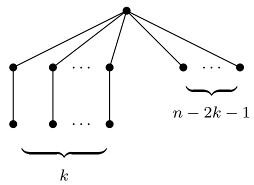

Figure 1. $S_{n,k}$

3. Upper bound for Zagrab indices of trees with given double Roman domination number

In this section, we provide upper bounds for the first and the second Zagreb indices of trees in terms of their double Roman domination number. First, we assume that γ_{dR} is an odd number. According to Lemma 3, $\Delta \leq n - \frac{\gamma_{dR}-1}{2}$. As a first result, we consider trees with the double Roman domination number γ_{dR} and the maximum degree $\Delta = n - \frac{\gamma_{dR}-1}{2}$.

Theorem 1. *Let T be a tree of order n and with the double Roman domination number γ_{dR}. If γ_{dR} is an odd number and $\Delta = n - \frac{\gamma_{dR}-1}{2}$, then $T = S_{n,\frac{\gamma_{dR}-3}{2}}$ and so*

$$M_1(T) = n^2 - (\gamma_{dR} - 2)n + \frac{1}{4}\gamma_{dR}^2 + \gamma_{dR} - \frac{21}{4};$$
$$M_2(T) = n^2 - \frac{\gamma_{dR}+1}{2}n + \frac{3}{2}\gamma_{dR} - \frac{7}{2}.$$

Proof. Let v be a vertex of degree Δ and $f : V(T) \to \{0,1,2,3\}$ be a function with the rule $f(v) = 3$, $f(N(v)) = 0$ and $f(V(T) \setminus N[v]) = 2$. Therefore

$$w(f) = 3 + 2(n - \Delta - 1) = 3 + 2(\frac{\gamma_{dR} - 1}{2} - 1) = \gamma_{dR}$$

and hence f is a γ_{dR}-function. Next, we claim that every neighbor of v has degree at most 2. To the contrary, suppose there exists $x \in N(v)$ with $d(x) \geq 3$. Clearly, the function $g : V(T) \to \{0,1,2,3\}$ defined by $g(x) = 3$, $g(N(x) - v) = 0$ and $g(z) = f(z)$ otherwise, is a DRDF of T with $w(g) = w(f) + 3 - 2(d(x) - 1) < w(f)$, a contradiction. Also, it can be seen that for every $u \notin N[v]$, $d(u) = 1$. This is because that if there exists some $y \in V(T)$ with $d(y, v) \geq 2$ and $d(y) \geq 2$, then the function $h : V(T) \to \{0,1,2,3\}$ defined by $h(y) = 3$, $h(N(y)) = 0$ and $h(z) = f(z)$ otherwise, is a DRDF of T with $w(h) \leq w(f) + 1 - 2(d(x) - 1) < w(f)$, a contradiction. Thus $T = S_{n,k}$ with $\Delta = n - k - 1$ and consequently $n - k - 1 = n - \frac{\gamma_{dR}-1}{2}$. So $k = \frac{\gamma_{dR}-3}{2}$ and hence $T = S_{n,\frac{\gamma_{dR}-3}{2}}$. This implies that

$$\begin{aligned} M_1(T) &= (n - \frac{\gamma_{dR} - 1}{2})^2 + 4(\frac{\gamma_{dR} - 3}{2}) + (n - \frac{\gamma_{dR} - 1}{2}) = n^2 - (\gamma_{dR} - 2)n + \frac{1}{4}\gamma_{dR}^2 + \gamma_{dR} - \frac{21}{4}; \\ M_2(T) &= \frac{\gamma_{dR} - 3}{2} \times (n - \frac{\gamma_{dR} - 1}{2}) \times 2 + \frac{\gamma_{dR} - 3}{2} \times 2 \times 1 + (n - \gamma_{dR} + 2) \times (n - \frac{\gamma_{dR} - 1}{2}) \times 1 \\ &= n^2 - \frac{\gamma_{dR} + 1}{2}n + \frac{3}{2}\gamma_{dR} - \frac{7}{2} \end{aligned}$$

and we are done. □

In the following theorem, we state an upper bound for the Zagreb indices of trees in term of γ_{dR}, in the case γ_{dR} is an odd number.

Theorem 2. *Let T be a tree of order n and with the double Roman domination number γ_{dR}. If γ_{dR} is an odd number, then*

$$\begin{aligned} M_1(T) &\leq n^2 - (\gamma_{dR} - 2)n + \frac{1}{4}\gamma_{dR}^2 + \gamma_{dR} - \frac{21}{4}; \\ M_2(T) &\leq n^2 - \frac{\gamma_{dR} + 1}{2}n + \frac{3}{2}\gamma_{dR} - \frac{7}{2}, \end{aligned}$$

and each equality holds if only if $T = S_{n,\frac{\gamma_{dR}-3}{2}}$.

Proof. We proceed the proof by induction on $diam(T)$. If $diam(T) = 1$, then $T = P_2 \cong S_{2,0}$ and whenever $diam(T) = 2$, then $T = S_n \cong S_{n,0}$. Therefore by Theorem 1 the result is clearly established. Now, assume that the theorem holds for all graphs with diameter less than d and consider T as a tree with diameter d. If $\Delta = n - \frac{\gamma_{dR}-1}{2}$, then by Theorem 1 the result holds. Therefore, let $\Delta < n - \frac{\gamma_{dR}-1}{2}$ and $P : x_1x_2 \cdots x_{d+1}$ be a diametrical path in T. We consider the following cases.

Case 1. If $d(x_2) \geq 4$, then x_2 has at least three leaves. Therefore, it can be shown that in this case $\gamma_{dR}(T') = \gamma_{dR}(T)$ where $T' = T \setminus \{x_1\}$. Thus by the induction hypothesis we have:

$$\begin{aligned}
M_1(T) &= M_1(T') + 2d(x_2)\\
&\leq (n-1)^2 - (\gamma_{dR} - 2)(n-1) + \frac{1}{4}\gamma_{dR}^2 + \gamma_{dR} - \frac{21}{4} + 2d(x_2)\\
&= n^2 - (\gamma_{dR} - 2)n + \frac{1}{4}\gamma_{dR}^2 + \gamma_{dR} - \frac{21}{4} - 2(n - \frac{\gamma_{dR} - 1}{2}) + 2d(x_2)\\
&< n^2 - (\gamma_{dR} - 2)n + \frac{1}{4}\gamma_{dR}^2 + \gamma_{dR} - \frac{21}{4},
\end{aligned}$$

and

$$\begin{aligned}
M_2(T) &= M_2(T') + \sum\nolimits_{y \in N[x_2]} d(y) - 1\\
&\leq (n-1)^2 - \frac{\gamma_{dR}+1}{2}(n-1) + \frac{3}{2}\gamma_{dR} - \frac{7}{2} + 2(n-1) - \sum\nolimits_{y \notin N[x_2]} d(y) - 1\\
&\leq n^2 - \frac{\gamma_{dR}+1}{2}n + \frac{3}{2}\gamma_{dR} - \frac{7}{2} - 2n + 1 + \frac{\gamma_{dR}+1}{2} + 2(n-1) - (n-1-d(x_2)) - 1\\
&= n^2 - \frac{\gamma_{dR}+1}{2}n + \frac{3}{2}\gamma_{dR} - \frac{7}{2} - (n - \frac{\gamma_{dR}-1}{2}) + d(x_2)\\
&< n^2 - \frac{\gamma_{dR}+1}{2}n + \frac{3}{2}\gamma_{dR} - \frac{7}{2}.
\end{aligned}$$

Case 2. If $d(x_2) = 3$, then $\gamma_{dR}(T) - 1 \leq \gamma_{dR}(T') \leq \gamma_{dR}(T)$.

Subcase 2-1. If $\gamma_{dR}(T') = \gamma_{dR}(T)$, then similar to Case 1, one can see that the desired inequalities hold strictly.

Subcase 2-2. If $\gamma_{dR}(T') = \gamma_{dR}(T) - 1$, then

$$\begin{aligned}
M_1(T) &= M_1(T') + 6\\
&\leq (n-1)^2 - (\gamma_{dR} - 3)(n-1) + \frac{1}{4}(\gamma_{dR} - 1)^2 + (\gamma_{dR} - 1) - \frac{21}{4} + 6\\
&= n^2 - (\gamma_{dR} - 2)n + \frac{1}{4}\gamma_{dR}^2 + \gamma_{dR} - \frac{21}{4} - (n - \frac{\gamma_{dR} - 1}{2}) - \frac{9}{4} + 6.
\end{aligned}$$

On the other hand, $n - \frac{\gamma_{dR}-1}{2} > \Delta \geq 3$. Thus $n - \frac{\gamma_{dR}-1}{2} \geq 4$ and hence

$$M_1(T) < n^2 - (\gamma_{dR} - 2)n + \frac{1}{4}\gamma_{dR}^2 + \gamma_{dR} - \frac{21}{4}.$$

Also, by a computer computation one can see that for every tree T of order at most 7, the stated bound for $M_2(T)$ in the theorem is established. Now, let $n \geq 8$. We have:

$$\begin{aligned}
M_2(T) &= M_2(T') + \sum\nolimits_{y\in N[x_2]} d(y) - 1\\
&\le (n-1)^2 - \frac{\gamma_{dR}}{2}(n-1) + \frac{3}{2}(\gamma_{dR}-1) - \frac{7}{2} + (3 + d(x_3) + 1 + 1) - 1\\
&= n^2 - \frac{\gamma_{dR}+1}{2}n + \frac{3}{2}\gamma_{dR} - \frac{7}{2} - 2n + 1 + \frac{n}{2} + \frac{\gamma_{dR}}{2} - \frac{3}{2} + d(x_3) + 4\\
&= n^2 - \frac{\gamma_{dR}+1}{2}n + \frac{3}{2}\gamma_{dR} - \frac{7}{2} - (n - \frac{\gamma_{dR}-1}{2}) + d(x_3) - \frac{1}{2}n + 4\\
&< n^2 - \frac{\gamma_{dR}+1}{2}n + \frac{3}{2}\gamma_{dR} - \frac{7}{2}.
\end{aligned}$$

Case 3. Let $d(x_2) = 2$. If $\gamma_{dR}(T) < \gamma_{dR}(T') + 2$, then similar to Case 1 and Subcase 2-2, it can be shown that the desired inequalities strictly hold. So, let $\gamma_{dR}(T) = \gamma_{dR}(T') + 2$. Then

$$\begin{aligned}
M_1(T) &= M_1(T') + 4\\
&\le (n-1)^2 - (\gamma_{dR}-4)(n-1) + \frac{1}{4}(\gamma_{dR}-2)^2 + (\gamma_{dR}-2) - \frac{21}{4} + 4\\
&= n^2 - (\gamma_{dR}-2)n + \frac{1}{4}\gamma_{dR}^2 + \gamma_{dR} - \frac{21}{4}.
\end{aligned}$$

Furthermore, by the induction hypothesis, equality holds if and only if $T' = S_{n-1,\frac{\gamma_{dR}-5}{2}}$. If x_2 is a leaf of T' with distance 2 from the central vertex of T', then $\gamma_{dR}(T) = \gamma_{dR}(T') + 1$ and we showed that in this case the inequality is strict. Therefore x_2 is one of the leaves of T' that adjacent to the central vertex of T' and consequently $T = S_{n,\frac{\gamma_{dR}-3}{2}}$. Also,

$$\begin{aligned}
M_2(T) &= M_2(T') + \sum\nolimits_{y\in N[x_2]} d(y) - 1\\
&\le (n-1)^2 - \frac{\gamma_{dR}-1}{2}(n-1) + \frac{3}{2}(\gamma_{dR}-2) - \frac{7}{2} + (2 + d(x_3) + 1) - 1\\
&= n^2 - \frac{\gamma_{dR}+1}{2}n + \frac{3}{2}\gamma_{dR} - \frac{7}{2} - (n - \frac{\gamma_{dR}-1}{2}) + d(x_3)\\
&< n^2 - \frac{\gamma_{dR}+1}{2}n + \frac{3}{2}\gamma_{dR} - \frac{7}{2}
\end{aligned}$$

and the results follow. □

Now, we consider trees with an even double Roman domination number. Let v be a vertex of T with $d(v) = \Delta$. Since γ_{dR} is even, there exists leaf $u \in V(T)$ with $d(u, v) \ge 3$. So, the function $f : V(T) \to \{0, 1, 2, 3\}$ defined by $f(u) = f(v) = 3$, $f(N(v)) = f(N(u)) = 0$ and $f(z) = 0$ otherwise, is a DRDF of T with $w(f) = 6 + 2(n - \Delta - 3) = 2n - 2\Delta$. It concludes that $\gamma_{dR} \le 2n - 2\Delta$ and consequently $\Delta \le n - \frac{\gamma_{dR}}{2}$. In the following, we examine trees with $\Delta = n - \frac{\gamma_{dR}}{2}$ and compute their Zagreb indices.

Theorem 3. *Let T be a tree of order n and with the double Roman domination number γ_{dR}. If γ_{dR} is an even number and $\Delta(T) = n - \frac{\gamma_{dR}}{2}$, then T is one of the following trees:*

$$S_{n-3,\frac{\gamma_{dR}-6}{2}} \bigoplus_{v,x_2} P_3 \quad , \quad S_{n-3,\frac{\gamma_{dR}-6}{2}} \bigoplus_{v,x_3} P_3 \quad , \quad S_{n-4,\frac{\gamma_{dR}-8}{2}} \bigoplus_{v,x_3} P_4$$

In particular, in the first case we have

$$M_1(T) = n^2 - (\gamma_{dR} - 1)n + \frac{1}{4}\gamma_{dR}^2 + \frac{3}{2}\gamma_{dR} - 2$$
$$M_2(T) = n^2 - \frac{\gamma_{dR}}{2}(n-3) - n;$$

and in the second case

$$M_1(T) = n^2 - (\gamma_{dR} - 1)n + \frac{1}{4}\gamma_{dR}^2 + \frac{3}{2}\gamma_{dR} - 4$$
$$M_2(T) = n^2 - \frac{\gamma_{dR}}{2}(n-3) - n - (n - \frac{\gamma_{dR}}{2});$$

and in the last case

$$M_1(T) = n^2 - (\gamma_{dR} - 1)n + \frac{1}{4}\gamma_{dR}^2 + \frac{3}{2}\gamma_{dR} - 2$$
$$M_2(T) = n^2 - \frac{\gamma_{dR}}{2}(n-3) - n - (n - \frac{\gamma_{dR}}{2}) + 3.$$

Proof. Let $v \in V(T)$ be a vertex of degree Δ. First note that if all other vertices of T are adjacent to v, then $T = S_n$ and $\gamma_{dR}(T) = 3$, a contradiction. We prove the theorem in the following cases.

Case 1. The eccentricity of v (i.e. the maximum distance of v and other vertices in T) is equal to 2. So, there exists a vertex x in the neighborhood of v with $d(x) \geq 3$. Because otherwise, $T = S_{n,k}$ and γ_{dR} is odd. In this case, we define $f : V(T) \to \{0, 1, 2, 3\}$ with the rule $f(v) = f(x) = 3$, $f(N(v) - \{x\}) = f(N(x) - \{v\}) = 0$ and $f(u) = 2$ otherwise. Therefore, f is a DRDF with

$$w(f) = 3 + 3 + 2[n - (\Delta + 1 + d(x) - 1)] = 2n - 2\Delta - 2d(x) + 6$$
$$= 2n - 2(n - \frac{\gamma_{dR}}{2}) - 2d(x) + 6 = \gamma_{dR} - 2d(x) + 6 \leq \gamma_{dR}$$

It concludes that $d(x) = 3$. Additionally, if there are two vertices x and y with $d(x) = d(y) = 3$, then by defining the function $g : V(T) \to \{0, 1, 2, 3\}$ with $g(v) = g(x) = g(y) = 3$, $g(N(v) - \{x, y\}) = g(N(x) - \{v\}) = g(N(y) - \{v\}) = 0$ and $g(z) = 2$ otherwise, we obtain a DRDF with

$$w(g) = 3 + 3 + 3 + 2(n - \Delta - 5) = 2n - 2\Delta - 1 = \gamma_{dR} - 1,$$

which is also a contradiction. Thus, $S_{n-3,\frac{\gamma_{dR}-6}{2}} \bigoplus_{v,x_2} P_3$.

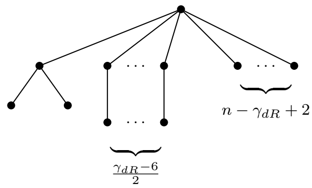

Figure 2. $S_{n-3,\frac{\gamma_{dR}-6}{2}} \bigoplus_{v,x_2} P_3$

Hence

$$\begin{aligned}
M_1(T) &= (n-\frac{\gamma_{dR}}{2})^2+9+4\times\frac{\gamma_{dR}-6}{2}+(n-\frac{\gamma_{dR}}{2}+1)\\
&= n^2-(\gamma_{dR}-1)n+\frac{1}{4}\gamma_{dR}^2+\frac{3}{2}\gamma_{dR}-2;\\
M_2(T) &= 3+3+3(n-\frac{\gamma_{dR}}{2})+(\gamma_{dR}-6)(n-\frac{\gamma_{dR}}{2})+(\gamma_{dR}-6)+(n-\gamma_{dR}+2)(n-\frac{\gamma_{dR}}{2})\\
&= n^2-\frac{\gamma_{dR}}{2}(n-3)-n = n^2-(1+\frac{\gamma_{dR}}{2})n+\frac{3}{2}\gamma_{dR}
\end{aligned}$$

Case 2. The eccentricity of v is equal to 3.
Subcase 2-1. If $d(u) \leq 2$ for any $u \in V(T)-\{v\}$, then T is isomorphic to the following tree.

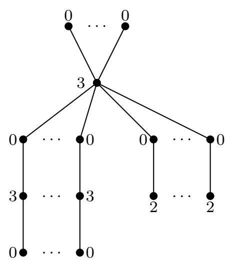

Figure 3. **The eccentricity of v is equal to 3.**

Consider $f: V(T) \to \{0,1,2,3\}$ with the rule $f(v)=3$, $f(N(v))=0$ and $f(V(T)-N[v])=2$. Clearly, f is a DRDF with $w(T)=3+2(n-\Delta-1)=\gamma_{dR}+1$. Another labeling for the vertices of T is shown in Figure 3. If we denote the function generating this labeling by g, then g is a DRDF with $w(g)=w(f)-k$, where k is the number of leaves of T that the distance of them and v is equal to 3. Thus $k=1$ and so $T \cong S_{n-3,\frac{\gamma_{dR}-6}{2}} \bigoplus_{v,x_3} P_3$.

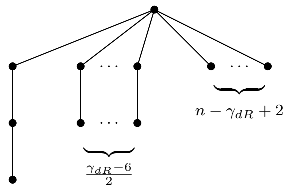

Figure 4. $S_{n-3,\frac{\gamma_{dR}-6}{2}} \bigoplus_{v,x_3} P_3$

So, we have

$$\begin{aligned}
M_1(T) &= (n-\frac{\gamma_{dR}}{2})^2 + 4(\frac{\gamma_{dR}-2}{2}) + (n-\frac{\gamma_{dR}}{2})\\
&= n^2 - (\gamma_{dR}-1)n + \frac{1}{4}\gamma_{dR}^2 + \frac{3}{2}\gamma_{dR} - 4;\\
M_2(T) &= 2+4+2(n-\frac{\gamma_{dR}}{2}) + (\gamma_{dR}-6)(n-\frac{\gamma_{dR}}{2}) + (\gamma_{dR}-6) + (n-\frac{\gamma_{dR}}{2})(n-\gamma_{dR}+2)\\
&= n^2 - \frac{\gamma_{dR}}{2}(n-3) - n - (n-\frac{\gamma_{dR}}{2})\\
&= n^2 - (2+\frac{\gamma_{dR}}{2})n + 2\gamma_{dR} = n^2 - (1+\frac{\gamma_{dR}}{2})n + \frac{3}{2}\gamma_{dR} - (n-\frac{\gamma_{dR}}{2}).
\end{aligned}$$

Subcase 2-2. If $d(x) \geq 3$ for some $x \in V(T) - \{v\}$, then we claim that $x \in N(v)$. To the contrary suppose $d(x,v) = 2$. Clearly, the function g with the rule $g(v) = g(x) = 3$, $g(N(v)) = g(N(x)) = 0$ and $g(z) = 2$ otherwise, is a DRDF with $w(g) = 6 + 2[n - (\Delta + d(x) + 1)] = \gamma_{dR} - 2d(x) + 4 < \gamma_{dR}$, a contradiction. So $x \in N(v)$ and the claim is proven. On the other hand, the function f that mentioned in Case 1 is a DRDF with $w(f) = \gamma_{dR} - 2d(x) + 6$. It concludes that $d(x) = 3$ and f is a γ_{dR}-function. Furthermore, x is a support vertex. Because otherwise there will be a DRDF with the weight $w(f) - 1$, a contradiction. Also, similar to the mentioned argument in Case 1, one can see that just one neighbor of v has degree 3. Finally, if there exists some $y \in V(T)$ such that $d(y,v) = d(y) = 2$ and $f(y) = 2$, then by changing the labels of y and its only adjacent leaf in f from 2 to 3 and 0 respectively, we obtain the DRDF with the weight $\gamma_{dR} - 1$ and this is a contradiction. Therefore $T \cong S_{n-4,\frac{\gamma_{dR}-8}{2}} \bigoplus_{v,x_3} P_4$.

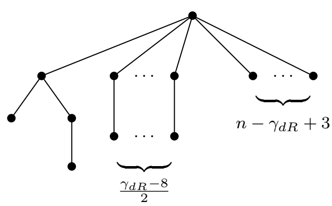

Figure 5. $S_{n-4,\frac{\gamma_{dR}-8}{2}} \bigoplus_{v,x_3} P_4$

So, we have

$$\begin{aligned}
M_1(T) &= (n-\frac{\gamma_{dR}}{2})^2+9+4(\frac{\gamma_{dR}-6}{2})+(n-\frac{\gamma_{dR}}{2}+1)\\
&= n^2-(\gamma_{dR}-1)n+\frac{1}{4}\gamma_{dR}^2+\frac{3}{2}\gamma_{dR}-2;\\
M_2(T) &= 3+2+6+3(n-\frac{\gamma_{dR}}{2})+(\gamma_{dR}-8)(n-\frac{\gamma_{dR}}{2})+(\gamma_{dR}-8)+(n-\gamma_{dR}+3)(n-\frac{\gamma_{dR}}{2})\\
&= n^2-\frac{\gamma_{dR}}{2}(n-4)-2n+3\\
&= n^2-(2+\frac{\gamma_{dR}}{2})n+2\gamma_{dR}+3 = n^2-(1+\frac{\gamma_{dR}}{2})n+\frac{3}{2}\gamma_{dR}-(n-\frac{\gamma_{dR}}{2})+3.
\end{aligned}$$

Case 3. The eccentricity of v is grater than 3. In this case, there exists a vertex x in T with $d(x)\geq 2$ and $d(x,v)=3$. So, by assigning 3 to x and v, zero to neighbors of x and v, and 2 to other vertices of T, we get a DRDF with the wight $\gamma_{dR}+2-2d(x)$, which is a contradiction. □

Here, we state an upper bound for the Zagreb indices of trees in term of γ_{dR}, in the case γ_{dR} is an even number.

Theorem 4. *Let T be a tree of order n and with the double Roman domination number γ_{dR}. If γ_{dR} is an even number, then*

$$\begin{aligned}
M_1(T) &\leq n^2-n(\gamma_{dR}-1)+\frac{1}{4}\gamma_{dR}^2+\frac{3}{2}\gamma_{dR}-2\\
M_2(T) &\leq n^2-(1+\frac{\gamma_{dR}}{2})n+\frac{3}{2}\gamma_{dR}.
\end{aligned}$$

The equalities hold for $T\in\{S_{n-3,\frac{\gamma_{dR}-6}{2}}\bigoplus_{v,x_2}P_3, S_{n-4,\frac{\gamma_{dR}-8}{2}}\bigoplus_{v,x_3}P_4\}$ and $T = S_{n-3,\frac{\gamma_{dR}-6}{2}}\bigoplus_{v,x_2}P_3$, respectively.

Proof. We proceed the proof by induction on $diam(T)$. First note that γ_{dR} is odd whenever $diam(T)\leq 2$. Now, let $diam(T)=3$. So, $T=DS_{p,q}$ and consequently $\gamma(T)=6$ (Note that due to γ_{dR} being even, $q\geq 2$). It concludes that

$$\begin{aligned}
M_1(DS_{p,q})-[n^2-(\gamma_{dR}-1)n+\frac{1}{4}\gamma_{dR}^2+\frac{3}{2}\gamma_{dR}-2] &= 4p+4q-2pq-8\leq 0\\
M_2(DS_{p,q})-[n^2-(1+\frac{\gamma_{dR}}{2})n+\frac{3}{2}\gamma_{dR}] &= 2p+2q-pq-4\leq 0
\end{aligned}$$

and each equality holds if and only if $T=DS_{p,2}\cong S_{n-3,0}\bigoplus_{v,x_2}P_3$. Next, assume that the theorem holds for all graphs with diameter less than d and and consider T as a tree with diameter $d\geq 4$. If $\Delta = n-\frac{\gamma_{dR}}{2}$, then by Theorem 3 the result holds. Therefore, let $\Delta < n-\frac{\gamma_{dR}}{2}$,$v_1v_2\cdots v_{d+1}$ be a diametral path in T and $T'=T\setminus\{v_1\}$. We consider the following cases:

Case 1. If $\gamma_{dR}(T)=\gamma_{dR}(T')$, then by the induction hypothesis we have:

$$\begin{aligned}M_1(T) &= M_1(T')+2d(v_2)\\ &\le (n-1)^2-(\gamma_{dR}-1)(n-1)+\frac{1}{4}\gamma_{dR}^2+\frac{3}{2}\gamma_{dR}-2+2d(v_2)\\ &= n^2-(\gamma_{dR}-1)n+\frac{1}{4}\gamma_{dR}^2+\frac{3}{2}\gamma_{dR}-2-2(n-\frac{\gamma_{dR}}{2})+2d(v_2)\\ &< n^2-(\gamma_{dR}-1)n+\frac{1}{4}\gamma_{dR}^2+\frac{3}{2}\gamma_{dR}-2,\end{aligned}$$

and

$$\begin{aligned}M_2(T) &= M_2(T')+\sum\nolimits_{u\in N[v_2]} d(u)-1\\ &\le (n-1)^2-(1+\frac{\gamma_{dR}}{2})(n-1)+\frac{3}{2}\gamma_{dR}+2(n-1)-\sum\nolimits_{u\notin N[v_2]} d(u)-1\\ &\le n^2-(1+\frac{\gamma_{dR}}{2})n+\frac{3}{2}\gamma_{dR}+\frac{\gamma_{dR}}{2}+2(n-1)-(n-1-d(v_2))-1\\ &= n^2-(1+\frac{\gamma_{dR}}{2})n+\frac{3}{2}\gamma_{dR}-(n-\frac{\gamma_{dR}}{2})+d(v_2)\\ &< n^2-(1+\frac{\gamma_{dR}}{2})n+\frac{3}{2}\gamma_{dR}.\end{aligned}$$

Case 2. If $\gamma_{dR}(T)=\gamma_{dR}(T')+1$, then by the induction hypothesis we have:

$$\begin{aligned}M_1(T) &= M_1(T')+2d(v_2)\\ &\le (n-1)^2-(\gamma_{dR}-2)(n-1)+\frac{1}{4}(\gamma_{dR}-1)^2+\frac{3}{2}(\gamma_{dR}-1)-2+2d(v_2)\\ &= n^2-(\gamma_{dR}-1)n+\frac{1}{4}\gamma_{dR}^2+\frac{3}{2}\gamma_{dR}-2-(n-\frac{\gamma_{dR}}{2})-\frac{9}{4}+2d(v_2)\\ &< n^2-(\gamma_{dR}-1)n+\frac{1}{4}\gamma_{dR}^2+\frac{3}{2}\gamma_{dR}-2.\end{aligned}$$

Also, $n-\frac{\gamma_{dR}}{2}\ge d(v_2)+1$. Hence $(n-\frac{\gamma_{dR}}{2})+\frac{9}{4}-2d(v_2)\ge\frac{13}{4}-d(v_2)$. On the other hand, $\gamma_{dR}(T)=\gamma_{dR}(T')+1$ implies that $d(v_2)\le 3$. So,

$$M_1(T)<n^2-(\gamma_{dR}-1)n+\frac{1}{4}\gamma_{dR}^2+\frac{3}{2}\gamma_{dR}-2.$$

Also, by a computer computation one can see that for every tree T of order at most 7, the stated bound for $M_2(T)$ in the theorem is established. Now, let $n\ge 8$. We have:

$$\begin{aligned}
M_2(T) &= M_2(T') + \sum\nolimits_{u\in N[v_2]} d(u) - 1\\
&\le (n-1)^2 - (1+\frac{\gamma_{dR}-1}{2})(n-1) + \frac{3}{2}(\gamma_{dR}-1) + (d(v_2)+d(v_3)+\overbrace{1+\cdots+1}^{(d(v_2)-1)\text{-times}}) - 1\\
&= n^2 - (1+\frac{\gamma_{dR}}{2})n + \frac{3}{2}\gamma_{dR} - (n-\frac{\gamma_{dR}}{2}) + d(v_3) - \frac{n}{2} + 2d(v_2) - 2\\
&< n^2 - (1+\frac{\gamma_{dR}}{2})n + \frac{3}{2}\gamma_{dR}.
\end{aligned}$$

Case 3. If $\gamma_{dR}(T) = \gamma_{dR}(T') + 2$, then $d(v_2) = 2$ and so

$$\begin{aligned}
M_1(T) &= M_1(T') + 4\\
&\le (n-1)^2 - (\gamma_{dR}-3)(n-1) + \frac{1}{4}(\gamma_{dR}-2)^2 + \frac{3}{2}(\gamma_{dR}-2) - 2 + 4\\
&= n^2 - (\gamma_{dR}-1)n + \frac{1}{4}\gamma_{dR}^2 + \frac{3}{2}\gamma_{dR} - 2.
\end{aligned}$$

Furthermore, by the induction hypothesis, equality holds if and only if either $T' = S_{n-4,\frac{\gamma_{dR}-8}{2}} \bigoplus_{v,x_2} P_3$ or $S_{n-5,\frac{\gamma_{dR}-10}{2}} \bigoplus_{v,x_3} P_4$. By considering the equation $\gamma_{dR}(T) = \gamma_{dR}(T') + 2$, if $T' = S_{n-4,\frac{\gamma_{dR}-8}{2}} \bigoplus_{v,x_2} P_3$, then $T = S_{n-3,\frac{\gamma_{dR}-6}{2}} \bigoplus_{v,x_2} P_3$ or $T' = S_{n-4,\frac{\gamma_{dR}-8}{2}} \bigoplus_{v,x_3} P_4$ and if $T' = S_{n-5,\frac{\gamma_{dR}-10}{2}} \bigoplus_{v,x_3} P_4$, then $T = S_{n-4,\frac{\gamma_{dR}-8}{2}} \bigoplus_{v,x_3} P_4$. Also,

$$\begin{aligned}
M_2(T) &= M_2(T') + \sum\nolimits_{u\in N[v_2]} d(u) - 1\\
&\le (n-1)^2 - (1+\frac{\gamma_{dR}-2}{2})(n-1) + \frac{3}{2}(\gamma_{dR}-2) + (2+d(v_3)+1) - 1\\
&= n^2 - (1+\frac{\gamma_{dR}}{2})n + \frac{3}{2}\gamma_{dR} - (n-\frac{\gamma_{dR}}{2}) + d(v_3)\\
&< n^2 - (1+\frac{\gamma_{dR}}{2})n + \frac{3}{2}\gamma_{dR}
\end{aligned}$$

and the proof is complete. □

4. Lower bound for the Zagrab indices of trees with given double Roman domination number

In this section, we provide lower bounds for the Zagreb indices of trees using their double Roman domination number.

Theorem 5. *Let T be a tree of order n and with the double Roman domination number γ_{dR}. Then $M_1(T) \ge 5n - \gamma_{dR} - 6$ and $M_2(T) \ge 5n - \gamma_{dR} - 8$. The first equality holds if only if $T = P_{3k}$ and the second equality holds if and only if $T = S_4$ or $T = P_{3k}$.*

Proof. First note that the results hold for $T = P_n$, by Lemmas 1 and 2. Moreover, if any two arbitrary leaves of T have distance 2, then $T = S_n$ and therefore

$$M_1(S_n) = (n-1)^2 + (n-1) = n^2 - n \geq 5n - 3 - 6 = 5n - 9.$$

Because, $(n-3)^2 = n^2 - 6n + 9 \geq 0$ and the equality holds if and only if $n = 3$ if and only if $T = P_3$. Also,

$$M_2(S_n) = (n-1)^2 = n^2 - 2n + 1 \geq 5n - 3 - 8 = 5n - 11.$$

Because, $n^2 - 7n + 12 \geq 0$ for $n \geq 3$ and the equality holds if and only if $n = 3, 4$ if and only if $T = P_3$ or $T = S_4$. Now, we assume $T \ncong P_n, S_n$ and consider two arbitrary leaves u and v in $V(T)$ with $d(u, v) \geq 3$. We proceed the proof by induction on n. Assume that $P : u = x_1 x_2 \cdots x_k = v$ is a unique path from u to v. We consider the following three cases.

Case 1. $d(x_2) \geq 3$. Let $T' = T - \{u\}$. Since $\gamma_{dR}(T') \leq \gamma_{dR}(T)$, we have

$$\begin{aligned} M_1(T) &= M_1(T') + 2d(x_2) \\ &\geq 5(n-1) - \gamma_{dR}(T') - 6 + 2d(x_2) \\ &\geq 5n - \gamma_{dR}(T) - 6 + 2d(x_2) - 5 \\ &> 5n - \gamma_{dR}(T) - 6. \end{aligned}$$

Also,

$$M_2(T) = M_2(T') + d(x_2) + \sum_{\substack{w \in N(x_2) \\ w \neq x_1}} N(x_2) = d(x_2) + d(x_3) + \sum_{\substack{w \in N(x_2) \\ w \neq x_1, x_3}} N(x_2) \geq 3 + 2 + 1 = 6.$$

It concludes that

$$M_2(T) \geq M_2(T') + 6 \geq 5(n-1) - \gamma_{dR}(T') - 8 + 6 > 5n - \gamma_{dR}(T) - 8.$$

Case 2. $d(x_2) = 2$ and $d(x_3) \geq 3$. Suppose T' is the connected component of T resulting from removing $x_2 x_3$ which contains x_3. Therefore, we have:

$$\begin{aligned} M_1(T) &= M_1(T') + d^2(x_3) - (d(x_3) - 1)^2 + 4 + 1 \\ &= M_1(T') + 2d(x_3) + 4 \\ &\geq 5(n-2) - \gamma_{dR}(T') - 6 + 2d(x_3) + 4 \\ &\geq 5n - \gamma_{dR}(T) - 6 + 2d(x_3) - 6 \quad (\text{Since} \gamma_{dR}(T') \leq \gamma_{dR}(T)) \\ &\geq 5n - \gamma_{dR}(T) - 6, \end{aligned}$$

and the equality holds if $T' = P_{n-2}$, $3|n-2$, $d(x_3) = 3$ and $\gamma_{dR}(T') = \gamma_{dR}(T)$. But, it is not hard to check that $\gamma_{dR}(P_{n-2} \bigoplus_{y,z} P_2) \neq \gamma_{dR}(P_{n-2})$ for all non-leaf vertices of P_{n-2}. Therefore, in this case as well, equality does not hold.
Also,

$$M_2(T) = M_2(T') + \sum_{\substack{w\in N(x_3)\\ w\neq x_2}} d(w) + 2d(x_3) + 2 \leq (1+1) + 6 + 2 = 10$$

and hence

$$M_2(T) \geq M_2(T') + 10 \geq 5(n-2) - \gamma_{dR}(T') - 8 + 10 = 5n - \gamma_{dR}(T) - 8.$$

Moreover, if the equality holds, then $d(x_3) = 3$ and $N(x_3) = \{x_2, x_4, y\}$ with $d(x_4) = d(y) = 1$. So, $T = DS_{2,1}$ and hence $M_2(T) = 14 > 12 = 5n - \gamma_{dR}(T) - 8$, a contradiction.

Case 3. Let $k \geq 4$ be the smallest index such that $d(x_k) \geq 3$ and T' be the connected component of T resulting from removing $x_{k-1}x_k$ which contains x_k. We have:

$$\begin{aligned} M_1(T) &= M_1(T') + d^2(x_k) - (d(x_k) - 1)^2 + 4(k-2) + 1 \\ &= M_1(T') + 2d(x_k) + 4k - 8 \\ &\geq 5(n-k+1) - \gamma_{dR}(T') - 6 + 2d(x_k) + 4k - 8. \end{aligned}$$

On the other hand, $\gamma_{dR}(T) \geq \gamma_{dR}(T') + \gamma_{dR}(P_{k-2})$ and hence $\gamma_{dR}(T') \leq \gamma_{dR}(T) - k + 2$, by Lemma 2. So,

$$\begin{aligned} M_1(T') &\geq 5n - \gamma_{dR}(T) - 6 + 2d(x_k) - 5 \\ &> 5n - \gamma_{dR}(T) - 6. \end{aligned}$$

Also,

$$\begin{aligned} M_2(T) &= M_2(T') + \sum_{\substack{w\in N(x_k)\\ w\neq x_{k-1}}} d(w) + 2d(x_k) + 4(k-2) + 2 \\ &\geq 5(n-k+1) - (\gamma_{dR}(T) - k + 2) - 8 + 2d(x_k) + 4k - 6 \\ &= 5n - \gamma_{dR}(T) - 8 + 2d(x_k) - 3 \\ &> 5n - \gamma_{dR}(T) - 8 \end{aligned}$$

and the results follow. □

5. Conclusion

The Zagreb indices - which introduced by Ivan Gutman and Nenad Trinajstić in 1972 - are a pair of parameters used in mathematical chemistry, specifically in the study of chemical compounds represented as graphs. They are calculated based on the degrees of vertices (number of connections) in a molecular graph. This paper is devoted to the investigation of relationship between the first and the second Zagreb indices and double Roman domination number of any arbitrary tree. More precisely, we establish upper and lower bounds of the first and the second Zagreb indices of trees in terms of their orders and double Roman domination numbers, and all the tree attaining the equality case are characterized.

Statements and Declarations

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References

[1] H.A. Ahangar, M. Chellali, and S.M. Sheikholeslami, *On the double Roman domination in graphs*, Discrete Appl. Math. **232** (2017), 1–7. https://doi.org/10.1016/j.dam.2017.06.014.

[2] A.A.S. Ahmad Jamri, R. Hasni, M. Kamran Jamil, and D.A. Mojdeh, *Maximum second Zagreb index of trees with given Roman domination number*, Trans. Comb. **12** (2023), no. 1, 1–10. https://doi.org/10.22108/toc.2022.128323.1848.

[3] A.A.S. Ahmad Jamri, R. Hasni, and S.K. Said Husain, *On the Zagreb indices of graphs with given Roman domination number*, Commun. Comb. Optim. **8** (2023), no. 1, 141–152. https://doi.org/10.22049/cco.2021.27439.1263.

[4] A.A.S. Ahmad Jamri, F. Movahedi, R. Hasni, and M.H. Akhbari, *A lower bound for the second Zagreb index of trees with given Roman domination number*, Commun. Comb. Cptim. **8** (2023), no. 2, 391–396. https://doi.org/10.22049/cco.2022.27553.1288.

[5] R.A. Beeler, T.W. Haynes, and S.T. Hedetniemi, *Double Roman domination*, Discrete Appl. Math. **211** (2016), 23–29. https://doi.org/10.1016/j.dam.2016.03.017.

[6] B. Borovićanin, K.C. Das, B. Furtula, and I. Gutman, *Bounds for Zagreb indices*, MATCH Commun. Math. Comput. Chem. **78** (2017), no. 1, 17–100.

[7] B. Borovićanin and B. Furtula, *On extremal Zagreb indices of trees with given domination number*, Appl. Math. Comput. **279** (2016), 208–218.
https://doi.org/10.1016/j.amc.2016.01.017.

[8] Z. Du, A.A.S. Ahmad Jamri, R. Hasni, and D.A. Mojdeh, *Maximal first Zagreb index of trees with given Roman domination number*, AIMS Maths. **7** (2021), no. 7, 11801–11812.
https://doi.org/10.3934/math.2022658.

[9] I. Gutman and K.C. Das, *The first Zagreb index 30 years after*, MATCH Commun. Math. Comput. Chem. **50** (2004), no. 1, 83–92.

[10] I. Gutman and N. Trinajstić, *Graph theory and molecular orbitals. Total π-electron energy of alternant hydrocarbons*, Chem. Phys. Lett. **17** (1972), no. 4, 535–538.
https://doi.org/10.1016/0009-2614(72)85099-1.

[11] N. Jafari Rad and H. Rahbani, *Some progress on the double Roman domination in graphs*, Discuss. Math. Graph Theory **39** (2018), no. 1, 41–53.
http://dx.doi.org/10.7151/dmgt.2069.

[12] D.A. Mojdeh, M. Habibi, L. Badakhshian, and Y. Rao, *Zagreb indices of trees, unicyclic and bicyclic graphs with given (total) domination*, IEEE Access **7** (2019), 94143–94149.
https://doi.org/10.1109/ACCESS.2019.2927288.

[13] S. Nikolić, G. Kovačević, A. Miličević, and N. Trinajstić, *The Zagreb indices 30 years after*, Croat. Chem. Acta. **76** (2003), no. 2, 113–124.